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Search Topic:

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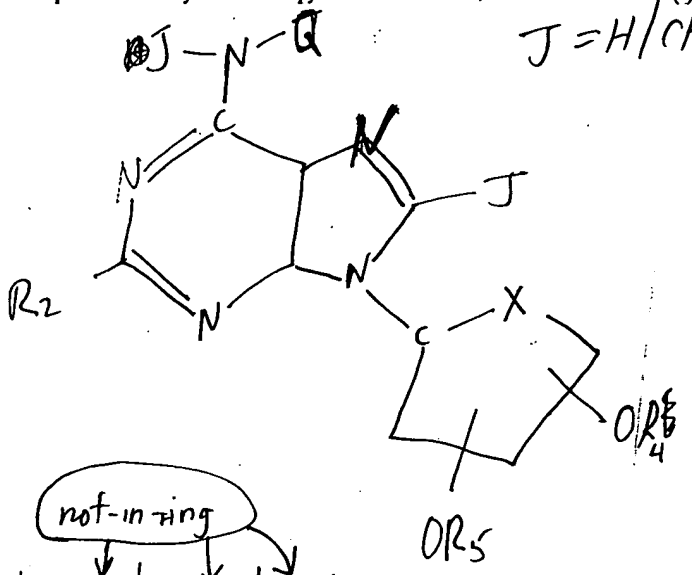
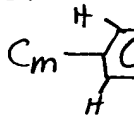
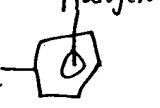


R_2 = H | Hal | O C | SC | C | SH; but not C_{1-5} alkyl

R_4, R_5 = H | C_{1-5} alkyl

X = O/S

Q = H | C_{1-5} alkyl | C_m  | CH_2 

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- ____ DARC/Questel
- ____ Other

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     FILE 'HCAPLUS' ENTERED AT 16:35:01 ON 25 MAR 2004
                  E JEONG L/AU
L22           109 S E3,E6-7
                  E LAK J/AU/AU
                  E LAK J/AU
                  E SHIN J/AU
                  E SHIN L/AU
                  E JACOBSON K/AU
L23           635 S E3-4,E22-27
                  E MOON H/AU
L24            39 E3 OR E17
                  E MOON HYONG/AU
                  E MOON HYUNG/AU
L25            67 S E3 OR E12-15
                  E KIM H/AU
L26           750 E3 OR E29
                  E KIM HEA/AU
L27            69 E7-8
L28             4 S L22-27 AND PURINE NUCLEOSIDE/TI

     FILE 'WPIX' ENTERED AT 16:44:18 ON 25 MAR 2004
                  E KIM H/AU
L29          5744 E3 OR E20
                  E MOON H/AU
L30           217 E3 OR E16
                  E JACOBSON K/AU
L31            51 E3-4
                  E JEONG L/AU
L32             9 S E3 OR E5
L33             0 S L29-32 AND PURINE NUCLEOSIDE/BIX
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FILE COVERS 1907 - 25 Mar 2004 VOL 140 ISS 13
FILE LAST UPDATED: 24 Mar 2004 (20040324/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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L28 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:674954 HCAPLUS
DN 136:53972
ED Entered STN: 14 Sep 2001
TI Synthesis and antiviral activity of D- and L-2'-azido-2',3'-dideoxy-4'-thiopyrimidine and **purine nucleosides**
AU **Jeong, Lak Shin**; Kim, Yun Ha; **Kim, Hea Ok**; Yoo, Su Jeong; Park, Yong Hee; Yeon, Sook Hee; Chun, Moon Woo; Kim, Hee-Doo
CS College of Pharmacy, Ewha Womans University, Seoul, S. Korea
SO Nucleosides, Nucleotides & Nucleic Acids (2001), 20(4-7), 665-668
CODEN: NNNAFY; ISSN: 1525-7770
PB Marcel Dekker, Inc.
DT Journal
LA English
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
AB Novel D- and L-2'-azido-2',3'-dideoxy-4'-thionucleosides were synthesized starting from L- and D-xylose via D- and L-4-thioarabitol derivative as key intermediates and evaluated for antiviral activity, resp. When the final nucleosides were tested against HIV-1, HSV-1, HSV-2, and HCMV, they were found to be only active against HCMV without cytotoxicity up to 100 μg/mL.
ST xylose thioarabitol intermediate prepn azido deoxy thiopyrimidine thiopurine nucleoside; herpesvirus HIV1 antiviral azido deoxy thiopyrimidine thiopurine nucleoside prepn
IT Antiviral agents
Cytotoxicity
Human herpesvirus 1
Human herpesvirus 2
Human herpesvirus 5
Human immunodeficiency virus 1
(preparation of D- and L-azido-thiopyrimidine or -purine nucleosides as potential antiviral agents)
IT Intermediates
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of D- and L-azido-thiopyrimidine or -purine nucleosides as potential antiviral agents using D- andL-4-thioarabitol derivative as key intermediates)
IT Nucleosides, preparation
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(thio; preparation of D- and L-azido-thiopyrimidine or -purine nucleosides as potential antiviral agents)
IT 335259-84-2P 335259-96-6P 335259-98-8P 335260-01-0P 335260-02-1P 335260-10-1P 335260-12-3P 335260-14-5P 335260-16-7P 335260-18-9P 335260-20-3P 335265-20-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of D- and L-azido-thiopyrimidine or -purine nucleosides as potential antiviral agents)
IT 58-86-6, D-Xylose, reactions 32865-86-4 85743-99-3 149712-85-6 149712-86-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of D- and L-azido-thiopyrimidine or -purine nucleosides as potential antiviral agents)
IT 20031-21-4P 218601-09-3P 218601-14-0P 218601-17-3P 335259-75-1P 335259-76-2P 335259-77-3P 335259-78-4P 335259-82-0P 335259-83-1P 335260-04-3P 335260-06-5P 335260-08-7P 381228-22-4P 381228-23-5P

381228-24-6P 381228-25-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of D- and L-azido-thiopyrimidine or -purine nucleosides as potential antiviral agents)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Dyson, M; J Med Chem 1991, V34, P2782 HCAPLUS
(2) Jeong, L; J Chem Soc, Perkin Trans 1 1998, V20, P3325
(3) Jeong, L; J Org Chem 1998, V63, P4821 HCAPLUS
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(5) Jeong, L; Tetrahedron Lett 1994, V35, P7573
(6) Nasr, M; Antiviral Res 1990, V14, P125 HCAPLUS
(7) Neyts, J; J Virol Methods 1991, V35, P27 HCAPLUS
(8) Rahim, S; J Med Chem 1996, V39, P789 HCAPLUS
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(12) van Draanen, N; J Med Chem 1996, V39, P789
(13) Yoshimura, Y; J Org Chem 1996, V61, P822 HCAPLUS

L28 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:316191 HCAPLUS
DN 133:83860
ED Entered STN: 16 May 2000
TI Methanocarba Analogues of **Purine Nucleosides** as Potent and Selective Adenosine Receptor Agonists
AU **Jacobson, Kenneth A.**; Ji, Xiao-duo; Li, An-Hu; Melman, Neli; Siddiqui, Maqbool A.; Shin, Kye-Jung; Marquez, Victor E.; Ravi, R. Gnana
CS Molecular Recognition Section Laboratory of Bioorganic Chemistry National Institute of Diabetes Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0810, USA
SO Journal of Medicinal Chemistry (2000), 43(11), 2196-2203
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 1-3 (Pharmacology)
Section cross-reference(s): 33
AB Adenosine receptor agonists have cardioprotective, cerebroprotective, and antiinflammatory properties. The authors report that a carbocyclic modification of the ribose moiety incorporating ring constraints is a general approach for the design of A1 and A3 receptor agonists having favorable pharmacodynamic properties. While simple carbocyclic substitution of adenosine agonists greatly diminishes potency, methanocarba-adenosine analogs have now defined the role of sugar puckering in stabilizing the active adenosine receptor-bound conformation and thereby have allowed identification of a favored isomer. In such analogs a fused cyclopropane moiety constrains the pseudosugar ring of the nucleoside to either a Northern (N) or Southern (S) conformation, as defined in the pseudorotational cycle. In binding assays at A1, A2A, and A3 receptors, (N)-methanocarba-adenosine was of higher affinity than the (S)-analog, particularly at the human A3 receptor (N/S affinity ratio of 150). (N)-methanocarba analogs of various N6-substituted adenosine derivs., including cyclopentyl and 3-iodobenzyl, in which the parent compds. are potent agonists at either A1 or A3 receptors, resp., were synthesized. The N6-cyclopentyl derivs. were A1 receptor-selective and maintained high efficacy at recombinant human but not rat brain A1 receptors, as indicated by stimulation of binding of [35S]GTP-γ-S. The (N)-methanocarba-N6-(3-iodobenzyl)adenosine and its 2-chloro derivative

had Ki values of 4.1 and 2.2 nM at A3 receptors, resp., and were highly selective partial agonists. Partial agonism combined with high functional potency at A3 receptors (EC50 < 1 nM) may produce tissue selectivity. In conclusion, as for P2Y1 receptors, at least three adenosine receptors favor the ribose (N)-conformation.

ST purine nucleoside methanocarba analog prepn adenosine agonist; adenosine receptor agonist purine nucleoside structure

IT Structure-activity relationship
(adenosine receptor-agonist; methanocarba analogs of purine nucleosides as potent and selective adenosine receptor agonists)

IT Purinoceptor agonists
(methanocarba analogs of purine nucleosides as potent and selective adenosine receptor agonists)

IT Adenosine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(methanocarba analogs of purine nucleosides as potent and selective adenosine receptor agonists)

IT 58-61-7, Adenosine, biological studies 37739-05-2 41552-82-3 163152-30-5 163152-31-6 281191-51-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(methanocarba analogs of purine nucleosides as potent and selective adenosine receptor agonists)

IT 174498-00-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(methanocarba analogs of purine nucleosides as potent and selective adenosine receptor agonists)

IT 281191-52-4P 281191-54-6P 281191-56-8P 281191-58-0P 281191-59-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(methanocarba analogs of purine nucleosides as potent and selective adenosine receptor agonists)

IT 1003-03-8, Cyclopentylamine 3718-88-5, 3-Iodobenzylamine hydrochloride 5451-40-1, 2,6-Dichloropurine 19186-33-5, Aristeromycin 49617-83-6, 3-Iodobenzyl bromide 281191-61-5 281191-66-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(methanocarba analogs of purine nucleosides as potent and selective adenosine receptor agonists)

IT 281191-63-7P 281191-64-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(methanocarba analogs of purine nucleosides as potent and selective adenosine receptor agonists)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(25) McVey, M; J Cardiovasc Pharmacol 1999, V33, P703 HCAPLUS
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(27) Moro, S; J Med Chem 1998, V41, P1456 HCAPLUS
(28) Nandanan, E; J Med Chem 2000, V43, P829 HCAPLUS
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(41) Yang, Q; Mol Pharmacol 1999, V56, P651 HCAPLUS

L28 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:292337 HCAPLUS
DN 133:150820
ED Entered STN: 05 May 2000
TI A highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-**purine nucleosides** as potential antiviral agents
AU **Kim, Hea Ok**; **Jeong, Lak Shin**; Lee, Sun Nan; Yoo, Soo Jeong; **Moon, Hyung Ryong**; Kim, Kil Soo; Chun, Moon Woo
CS College of Medicine, Yonsei University, Seoul, 120-752, S. Korea
SO Perkin 1 (2000), (9), 1327-1329
CODEN: PERKF9
PB Royal Society of Chemistry
DT Journal
LA English
CC 33-9 (Carbohydrates)
OS CASREACT 133:150820
AB L-β-2'-Deoxy-4'-thio-1'-purine nucleosides were synthesized efficiently utilizing the neighboring group effect of the 2-benzoyl-4-thiosugar acetate.
ST deoxythiopurine nucleoside prepn
IT Nucleosides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(thio; highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
IT 32865-86-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation with L-2-benzoyl-4-thiosugar acetate derivative; highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides

as potential antiviral agents)
IT 287725-04-6
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
IT 219662-00-7P 287724-97-4P 287724-98-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
IT 210548-19-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Mitsunobu benzoylation; highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
IT 287724-99-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Pummerer rearrangement and acetylation; highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
IT 287725-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and condensation with silylated 6-chloropurine; highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
IT 287725-03-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and debenzoylation with boron tribromide; highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
IT 287725-02-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deoxygenation; highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
IT 218601-09-3P 287725-01-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and selective debenzoylation; highly efficient synthesis of L-β-2'-deoxy-4'-thio-1'-purine nucleosides as potential antiviral agents)
RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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Cancer Chemotherapeutic Agents 1981, P229 HCAPLUS
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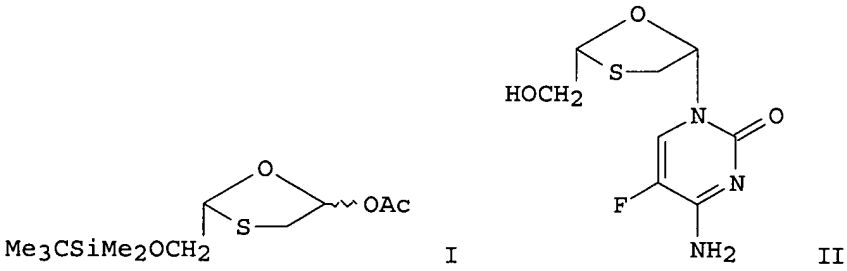
L28 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:124943 HCAPLUS
DN 118:124943
ED Entered STN: 30 Mar 1993
TI Asymmetric synthesis and biological evaluation of β-L-(2R,5S)- and α-L-(2R,5R)-1,3-oxathiolane-pyrimidine and - **purine nucleosides** as potential anti-HIV agents
AU **Jeong, Lak S.**; Schinazi, Raymond F.; Beach, J. Warren; **Kim, Hea O.**; Nampalli, Satyanarayana; Shanmuganathan, Kirupathevy; Alves, Antonio J.; McMillan, Angela; Chu, Chung K.; Mathis, Rodney
CS Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA
SO Journal of Medicinal Chemistry (1993), 36(2), 181-95
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1
GI



AB In order to study the structure-activity relationships of L-oxathiolanyl nucleosides as potential anti-HIV agents, a series of enantiomerically pure L-oxathiolanyl pyrimidine and purine nucleosides were synthesized and evaluated for anti-HIV-1 activity in human peripheral blood mononuclear (PBM) cells. The key intermediate I was synthesized starting from L-gulose via 1,6-thioanhydro-L-gulopyranose. I was condensed with thymine, 5-substituted uracils and cytosines, 6-chloropurine, and 6-chloro-2-fluoropurine to give pyrimidine and purine nucleosides. The 5-fluorocytosine derivative II was the most potent compound among those tested. In the case of 5-substituted cytosine analogs, the antiviral potency decreased in the order: cytosine (β-isomer) > 5-iodocytosine (β-isomer) > 5-fluorocytosine (α-isomer) > 5-methylcytosine (α-isomer) > 5-methylcytosine (β-isomer) > 5-bromocytosine (β-isomer) > 5-chlorocytosine (β-isomer). Among the thymine, uracil and 5-substituted uracil derivs. thymine (α-isomer) and uracil (β-isomer) derivs. exhibited moderate anti-HIV activity. In the purine series, the antiviral potency decreased in the order: adenine (β-isomer) > 6-chloropurine (β-isomer) > 6-chloropurine (α-isomer) > 2-amino-6-chloropurine (β-isomer) > guanine (β-isomer) > N6-methyladenine (α-isomer) > N6-methyladenine

(β-isomer). The cytotoxicity was also determined in human PBM and Vero cells. None of the synthesized nucleosides was toxic at ≤100 μM in PBM cells.

ST hydroxymethyloxathiolane nucleoside prepn virucide

IT Virucides and Virustats
(hydroxymethyloxathiolane nucleosides)

IT Nucleosides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(analogs, hydroxymethyloxathiolanyl, preparation and anti-HIV activity of)

IT Virus, animal
(human immunodeficiency 1, inhibitors, hydroxymethyloxathiolanyl nucleosides)

IT 145913-77-5P 145986-39-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)

IT 134678-17-4P 139757-68-9P 143491-57-0P 145913-75-3P 145913-76-4P
145913-80-0P 145913-82-2P 145986-07-8P 145986-08-9P 145986-09-0P
145986-10-3P 145986-11-4P 145986-12-5P 145986-13-6P 145986-14-7P
145986-15-8P 145986-16-9P 145986-17-0P 145986-18-1P 145986-24-9P
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145986-30-7P 145986-31-8P 145986-32-9P 145986-35-2P 145986-36-3P
145986-37-4P 145986-38-5P 145986-42-1P 145986-44-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and anti-HIV activity of)

IT 139757-69-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)

IT 139757-73-6P 139757-74-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deacetylation of)

IT 145913-78-6P 145913-79-7P 145986-40-9P 145986-41-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deblocking of)

IT 145913-64-0P 145913-65-1P 145913-66-2P 145913-67-3P 145913-68-4P
145913-69-5P 145913-70-8P 145913-71-9P 145913-72-0P 145913-73-1P
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145986-33-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of)

IT 145985-96-2P 145986-45-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and glycosidation by, of nucleic acid bases)

IT 139689-02-4P 139689-04-6P 139757-71-4P
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(preparation and oxidation of)

IT 139757-70-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
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IT 145913-74-2P 145986-34-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation, amination, and anti-HIV activity of)
IT 145913-81-1P 145986-43-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, hydrolysis, and anti-HIV activity of)
IT 139689-03-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, silylation, and deisopropylidenation of)
IT 1651-29-2, 2-Fluoro-6-chloropurine 14631-20-0, N-Acetylcytosine
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation and glycosidation of, by silyloxymethyloxathiolanyl acetate)
IT 87-42-3, 6-Chloropurine
RL: RCT (Reactant); RACT (Reactant or reagent)
(silylation and glycosidation of, with silyloxymethyloxathiolanyl acetate)
IT 51-20-7, 5-Bromouracil 51-21-8, 5-Fluorouracil 65-71-4 66-22-8, Uracil, reactions 696-07-1, 5-Iodouracil 1820-81-1, 5-Chlorouracil 10357-07-0, N4-Benzoyl-5-fluorocytosine 126354-30-1, N4-Benzoyl-5-methylcytosine 145913-83-3, N4-Benzoyl-5-chlorocytosine 145913-84-4, N4-Benzoyl-5-bromocytosine 145913-85-5, N4-Benzoyl-5-iodocytosine
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(silylation and reaction of, with silyloxymethyloxathiolanyl acetate)
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(silylation and reaction of, with silyloxymethyloxathiolanyl acetate)

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=> d his

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L7          19044 S L3 NOT L6
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L9          13755 S L8 FULL SUB=L7
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L13            50 S L12 CSS SAM SUB=L3
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L16               STR L15
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     FILE 'HCAPLUS' ENTERED AT 16:26:47 ON 25 MAR 2004
L19            15 S L18

     FILE 'USPATFULL, USPAT2' ENTERED AT 16:27:13 ON 25 MAR 2004
L20             1 S L18

     FILE 'HCAOLD' ENTERED AT 16:27:29 ON 25 MAR 2004
L21             0 S L18

     FILE 'HOME' ENTERED AT 16:29:21 ON 25 MAR 2004

=> b reg
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STRUCTURE FILE UPDATES:   24 MAR 2004  HIGHEST RN 667234-34-6
DICTIONARY FILE UPDATES:  24 MAR 2004  HIGHEST RN 667234-34-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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L2                STR
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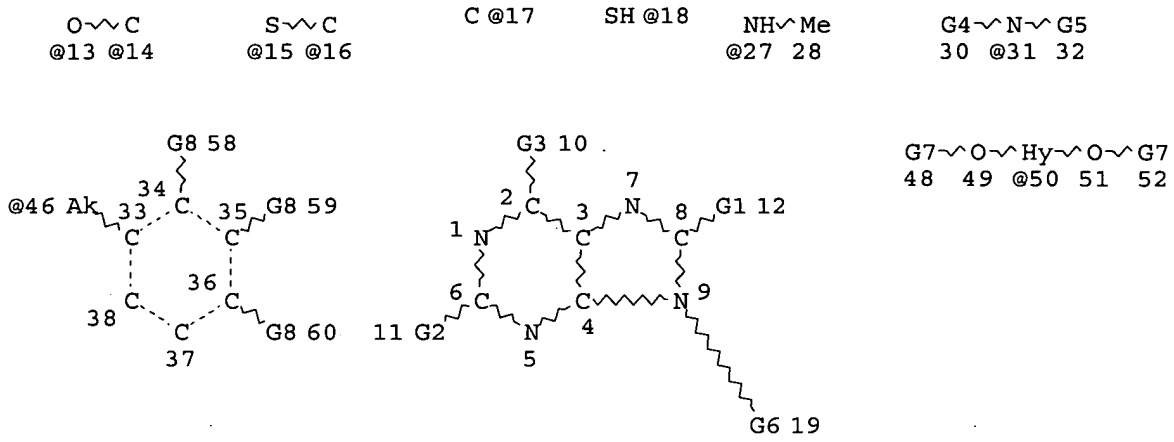

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VAR G7=H/AK
VAR G8=H/X
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NSPEC IS C AT 16
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GGCAT IS MCY AT 50
GGCAT IS MCY AT 55
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS E4 C E1 O AT 50
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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 44

STEREO ATTRIBUTES: NONE
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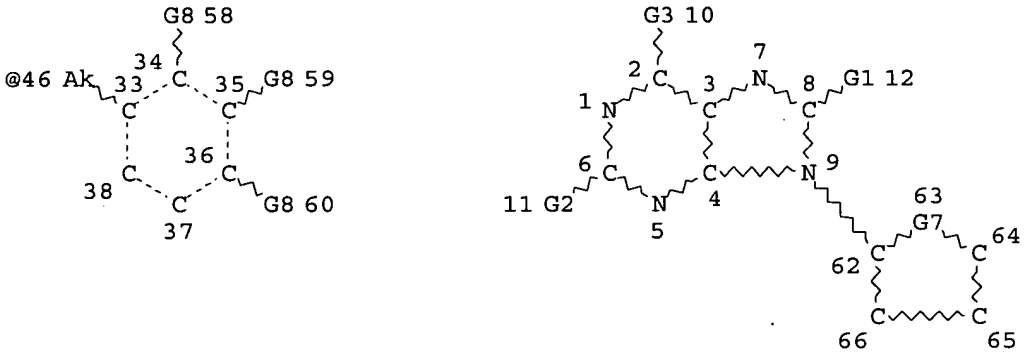

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STEREO ATTRIBUTES: NONE
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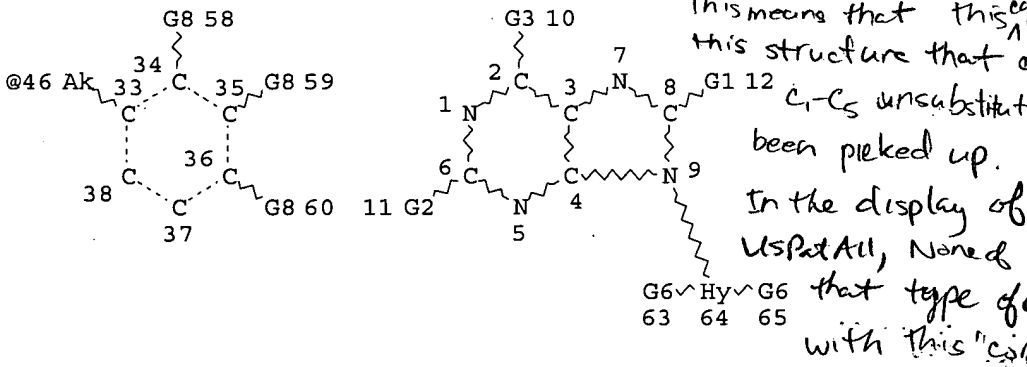

The connect on the highlighted carbon is a minimum of 1 substituent. This means that this carbon was the only place in this structure that could be substituted. C_1-C_5 unsubstituted alkyl chain could have been picked up.

In the display of results in HEAPlus and USPatAll, None of the hit structures had that type of chain. Therefore, no compounds with this "core ring structure and an unsubstituted carbon chain up to 5 carbons have not been made yet.

Searched by Noble Jarrell 272-2556

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VAR G2=H/X/S/13/15/17
VAR G3=NH2/27/31
VAR G4=H/ME
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100.0% PROCESSED  14613 ITERATIONS                          17 ANSWERS
SEARCH TIME: 00.00.01


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FILE LAST UPDATED: 24 Mar 2004  (20040324/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d all hitstr l19 tot

L19  ANSWER 1 OF 15  HCAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:1008314  HCAPLUS
DN   140:195030
ED   Entered STN:  29 Dec 2003
TI   Why does TNA cross-pair more strongly with RNA than with DNA? An answer
     from x-ray analysis
AU   Pallan, Pradeep S.; Wilds, Christopher J.; Wawrzak, Zdzislaw;
     Krishnamurthy, Ramanarayanan; Eschenmoser, Albert; Egli, Martin
CS   Department of Biochemistry, Vanderbilt University, Nashville, TN, 37332,
```

USA
SO Angewandte Chemie, International Edition (2003), 42(47), 5893-5895
CODEN: ACIEF5; ISSN: 1433-7851
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
CC 6-2 (General Biochemistry)
Section cross-reference(s): 33, 75
AB L-α-Threofuranosyl (3'→2') nucleic acid (TNA) residues adopt a C4'-exo pucker when incorporated into an A- or a B-form DNA duplex. The resulting intranucleotide P···P distance in TNA is very similar to that in RNA (represented by a C3'-endo puckered adenosine residue). The structural data explain earlier observations that TNA hybridizes more stably with RNA than with DNA and that RNA constitutes the better template for ligating TNA fragments.
ST threofuranosyl nucleic acid DNA duplex crystal structure; threofuranose conformation complexation DNA RNA
IT Conformation
Molecular association
(C4'-exo pucker conformation of α-L-threofuranosyladenosine in A-form DNA duplex in relation to relative hybridization with RNA and DNA)
IT DNA
RNA
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(C4'-exo pucker conformation of α-L-threofuranosyladenosine in A-form DNA duplex in relation to relative hybridization with RNA and DNA)
IT Crystal structure
(of A-form DNA duplex containing single α-L-threofuranosyladenosine residue)
IT **14266-03-6** 661494-47-9
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(C4'-exo pucker conformation of α-L-threofuranosyladenosine in A-form DNA duplex in relation to relative hybridization with RNA and DNA)
RE.CNT 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; http://www.rcsb.org
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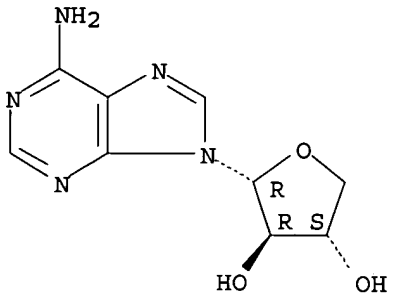
IT **14266-03-6**
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(C4'-exo pucker conformation of α-L-threofuranosyladenosine in A-form DNA duplex in relation to relative hybridization with RNA and DNA)
RN 14266-03-6 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, (2R,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:801947 HCAPLUS
DN 138:24912
ED Entered STN: 23 Oct 2002
TI Theoretical Study of 9-β-D-Erythrofuranosyladenine and Corresponding Carbocyclic Analogues. Evidence for a Base-Activated Conformational Lock
AU Akdag, Akin; Carver, Cynthia M.; McKee, Michael L.; Schneller, Stewart W.
CS Department of Chemistry, Auburn University, Auburn, AL, 36849, USA
SO Journal of Physical Chemistry A (2002), 106(46), 11254-11261
CODEN: JPCAFH; ISSN: 1089-5639
PB American Chemical Society
DT Journal
LA English
CC 33-9 (Carbohydrates)
Section cross-reference(s): 22
AB The conformational surfaces of three nucleoside analogs have been investigated computationally, where an adenine is attached to a diol of THF, a diol of cyclopentane, and a diol of cyclopentene. In each system, the lowest-energy conformer displays a conformational lock into the south position by an internal hydrogen bond between O2'H of the five-membered ring and the N3 nitrogen of adenine. When aqueous solvation is accounted for by the PCM method, the preference for the locked conformer is diminished. A pseudorotation angle of 9-(trans-2',trans-3'dihydroxycyclopentyl)adenine has been determined to be 176.8° by fitting the measured 3JHH values using PSEUROT which is in good agreement with the calculated value of 169.3°.
ST erythrofuranosyladenine nucleoside analog conformational analysis; adenine carbocyclic analog mol mechanics conformational analysis
IT Density functional theory
(B3LYP; ab initio and mol. mechanics study of 9-β-D-erythrofuranosyladenine and its carbocyclic analogs)
IT Conformational potential

Conformers
Molecular mechanics
(ab initio and mol. mechanics study of 9-β-D-erythrofuranosyladenine and its carbocyclic analogs)

IT Nucleoside analogs
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(ab initio and mol. mechanics study of 9-β-D-erythrofuranosyladenine and its carbocyclic analogs)

IT Hydrogen bond
(intramol.; ab initio and mol. mechanics study of 9-β-D-erythrofuranosyladenine and its carbocyclic analogs)

IT Molecular rotation
(pseudorotation; ab initio and mol. mechanics study of 9-β-D-erythrofuranosyladenine and its carbocyclic analogs)

IT Molecular vibration
(pseudorotational; ab initio and mol. mechanics study of 9-β-D-erythrofuranosyladenine and its carbocyclic analogs)

IT **17019-46-4** 111005-70-0 125409-63-4
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(ab initio and mol. mechanics study of 9-β-D-erythrofuranosyladenine and its carbocyclic analogs)

RE.CNT 98 THERE ARE 98 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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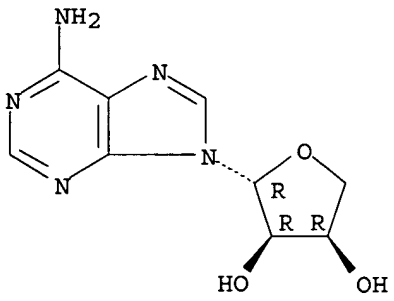
IT **17019-46-4**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)
(ab initio and mol. mechanics study of 9-β-D-erythrofuranosyladenine and its carbocyclic analogs)

RN 17019-46-4 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:59484 HCAPLUS
DN 130:252588
ED Entered STN: 29 Jan 1999
TI Biomimetic Simulation of Free Radical-Initiated Cascade Reactions Postulated To Occur at the Active Site of Ribonucleotide Reductases
AU Robins, Morris J.; Guo, Zhiqiang; Samano, Mirna C.; Wnuk, Stanislaw F.
CS Department of Chemistry and Biochemistry, Brigham Young University Provo, Provo, UT, 84602-5700, USA
SO Journal of the American Chemical Society (1999), 121(7), 1425-1433
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 33-9 (Carbohydrates)
Section cross-reference(s): 7

AB Treatment of 5'-O-nitro esters of nucleosides with tributylstannane and AIBN at elevated temps. caused β-scission of the resulting 5'-oxygen radical to give formaldehyde and dehomologated erythrofuranosyl nucleosides. Analogous treatment of 6'-O-nitro esters of homonucleosides [(5-deoxy-β-D-ribo-hexofuranosyl)adenine or uracil nucleosides derived from D-glucose] resulted in generation of a 6'-oxygen radical followed by abstraction of H3' by a [1,5]-hydrogen shift. Radical quenching with tributyltin deuteride gave 3'-[2H]-homonucleosides. This deuterium transfer, and inversion of configuration at C3' with unprotected homonucleosides, confirmed the relay-generation of C3' free radicals. Analogous treatment of 6'-O-nitro esters of homonucleosides containing a 2'-chloro or 2'-O-tosyl substituent resulted in complete disappearance of starting material and generation of (R)-2-(2-hydroxyethyl)-3(2H)-furanone (I). Generation of a 6'-oxygen radical, [1,5]-hydrogen shift of H3' to give a C3' radical, and loss of the 2'-substituent would give unstable intermediates that could lose the heterocyclic base from C1' to give I.

This radical-initiated cascade simulates reactions postulated to occur at the active site of ribonucleotide reductases. Generation of a C3' radical and loss of toluenesulfonic acid via a [1,2]-electron shift would generate a radical intermediate that could undergo deuterium transfer followed by β-elimination of the base to give the deuterated furanone I, as observed This is in harmony with a new mechanism for substrate reduction of nucleotides to give 2'-deoxy products. Generation of a C3' radical and loss of a chlorine atom by β-radical elimination would result in conjugate elimination of base and generation of I without incorporation of deuterium, as observed Thus, one-electron elimination processes (as well as the previously postulated two-electron loss with groups from C2') must be considered with mechanism-based inactivators of ribonucleotide reductases. Biomimetic reactions and new mechanistic considerations are discussed.

ST elimination radical ribonucleotide reductase active site simulation; ribonucleotide reductase active site nucleoside biomimetic; nucleoside biomimetic simulation free radical reaction

IT Enzyme functional sites
(active; biomimetic simulation of free radical-initiated cascade reactions postulated to occur at the active site of ribonucleotide reductases)

IT Elimination reaction
Simulation and Modeling, biological
(biomimetic simulation of free radical-initiated cascade reactions postulated to occur at the active site of ribonucleotide reductases)

IT Nucleosides, preparation
Radicals, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(biomimetic simulation of free radical-initiated cascade reactions postulated to occur at the active site of ribonucleotide reductases)

IT 9040-57-7, Ribonucleotide Reductase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(biomimetic simulation of free radical-initiated cascade reactions postulated to occur at the active site of ribonucleotide reductases)

IT 154-17-6 362-75-4 6001-17-8 18549-40-1 24807-96-3 31795-13-8 40635-66-3, α-Acetoxyisobutyryl chloride 52443-10-4 221671-02-9 221671-03-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(biomimetic simulation of free radical-initiated cascade reactions postulated to occur at the active site of ribonucleotide reductases)

IT 3253-91-6P 19684-32-3P 22415-88-9P 25577-41-7P 55085-28-4P 55085-32-0P 132587-37-2P 136523-39-2P 184045-08-7P 184045-09-8P 184045-10-1P 184045-11-2P 184045-12-3P 184045-13-4P 184045-14-5P 184045-15-6P 184181-19-9P 189165-93-3P 189165-94-4P 189165-95-5P 189165-96-6P 189165-98-8P 189166-00-5P 189166-01-6P 220325-36-0P 221670-83-3P 221670-84-4P 221670-87-7P 221670-91-3P 221670-92-4P 221670-93-5P 221670-96-8P 221670-97-9P 221670-98-0P 221670-99-1P 221671-01-8P 221671-04-1P 221671-05-2P 221671-06-3P 221671-07-4P 221671-08-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(biomimetic simulation of free radical-initiated cascade reactions postulated to occur at the active site of ribonucleotide reductases)

IT 30685-57-5P 30685-58-6P 67011-03-4P 109923-68-4P 184045-16-7P 184045-17-8P 221670-85-5P **221670-86-6P** 221670-88-8P 221670-89-9P 221670-90-2P 221670-94-6P 221670-95-7P 221671-00-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(biomimetic simulation of free radical-initiated cascade reactions postulated to occur at the active site of ribonucleotide reductases)

RE.CNT 87 THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS RECORD
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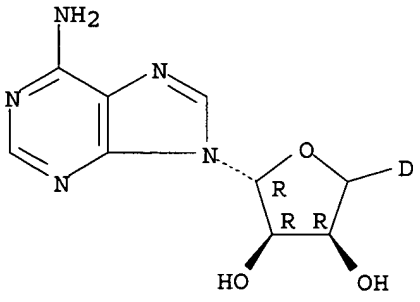
IT **221670-86-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(biomimetic simulation of free radical-initiated cascade reactions postulated to occur at the active site of ribonucleotide reductases)

RN 221670-86-6 HCAPLUS

CN 3,4-Furan-5-d-diol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, (2R,3R,4R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:329095 HCAPLUS
DN 129:75990
ED Entered STN: 03 Jun 1998
TI A functional screening of adenosine analogs at the adenosine A2B receptor:

a search for potent agonists

AU De Zwart, Maarten; Link, Regina; Von Frijtag Drabbe Kunzel, Jacobien K.; Cristalli, Gloria; Jacobson, Kenneth A.; Townsend-Nicholson, Andrea; Ijzerman, Ad P.

CS Division of Medicinal Chemistry, Leiden/Amsterdam Center for Drug Research, Leiden University, Leiden, 2300 RA, Neth.

SO Nucleosides & Nucleotides (1998), 17(6), 969-985
CODEN: NUNUD5; ISSN: 0732-8311

PB Marcel Dekker, Inc.

DT Journal

LA English

CC 1-3 (Pharmacology)

AB Various adenosine analogs were tested at the adenosine A2B receptor. Agonist potencies were determined by measuring the cAMP production in Chinese Hamster Ovary cells expressing human A2B receptors. 5'-N-Substituted carboxamidoadenosines were most potent. 5'-N-Ethylcarboxamidoadenosine (NECA) was most active with an EC50 value of 3.1 μM. Other ribose modified derivs. displayed low to negligible activity. Potency was reduced by substitution on the exocyclic amino function (N6) of the purine ring system. The most active N6-substituted derivative N6-methyl-NECA was 5 fold less potent than NECA. C8- and most C2-substituted analogs were virtually inactive. 1-Deaza-analogs had a reduced potency, 3- and 7-deazaanalogues were not active.

ST adenosine receptor agonist screening structure activity

IT Adenosine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(A2b; functional screening of adenosine analogs at adenosine A2B receptor: search for potent agonists)

IT Structure-activity relationship
(receptor-binding; functional screening of adenosine analogs at adenosine A2B receptor: search for potent agonists)

IT 58-61-7, Adenosine, biological studies 58-61-7D, Adenosine, analogs, biological studies 69-33-0 146-77-0 146-78-1 2620-62-4 3001-44-3
4294-16-0 5536-17-4 6736-58-9 14432-09-8 15397-13-4 17270-24-5
19186-33-5 20125-39-7 20649-47-2 23096-10-8 23589-16-4
23707-32-6 23707-33-7 24027-95-0 25030-31-3 35109-88-7
35868-16-7 35920-39-9, NECA 38594-96-6 41552-82-3 43157-47-7
43157-48-8 43157-50-2 50908-62-8 53296-10-9 56720-67-3
60687-65-2 60687-66-3 66822-83-1 72209-31-5 83683-90-3
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113628-10-7 137490-52-9 141585-94-6 143668-15-9 148527-87-1
150132-22-2 152540-76-6 152918-15-5 152918-17-7 152918-18-8
152918-19-9 152918-22-4 152918-23-5 152918-24-6 152918-25-7
152918-27-9 152918-30-4 152918-33-7 152918-34-8 152918-35-9
152918-36-0 152918-37-1 152918-38-2 152918-39-3 152918-40-6
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163152-31-6 163152-32-7 163152-33-8 163152-34-9 163259-24-3
199473-26-2 209337-22-4 209337-23-5 209337-24-6 209337-25-7
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209337-32-6 209337-33-7 209337-34-8
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(functional screening of adenosine analogs at adenosine A2B receptor: search for potent agonists)

IT 60-92-4, CAMP
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(functional screening of adenosine analogs at adenosine A2B receptor: search for potent agonists)

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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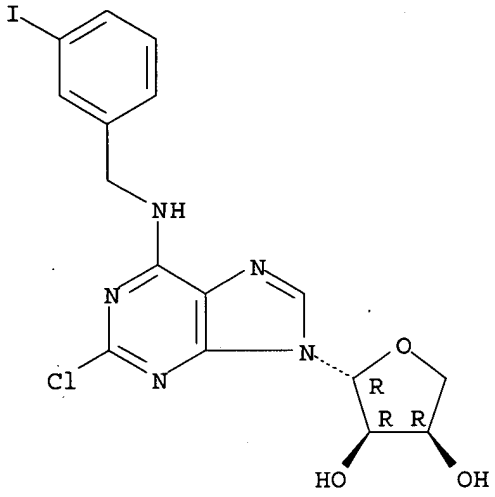
IT **163042-77-1**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(functional screening of adenosine analogs at adenosine A2B receptor: search for potent agonists)

RN 163042-77-1 HCAPLUS

CN 3,4-Furandiol, 2-[2-chloro-6-[[(3-iodophenyl)methyl]amino]-9H-purin-9-yl]tetrahydro-, (2R,3R,4R)- (9CI) (CA INDEX NAME)

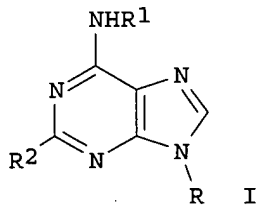
Absolute stereochemistry.



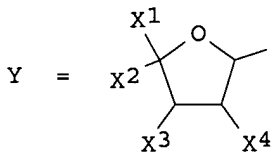
L19 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:761605 HCAPLUS
DN 128:34983
ED Entered STN: 06 Dec 1997
TI Preparation of nucleosides as A3 adenosine receptor agonists
IN Jacobson, Kenneth A.; Jeong, Heaok Kim; Siddiqi, Suhaib M.; Johnson, Carl R.; Secrist, John A., III; Tiwari, Kamal N.
PA United States Dept. of Health and Human Services, USA
SO U.S., 35 pp., Cont.-in-part of U.S. Ser. No. 274,628.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-70
ICS C07H019-167; C07H019-173
NCL 514046000
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5688774	A	19971118	US 1995-396111	19950228
	US 5773423	A	19980630	US 1994-274628	19940713
PRAI	US 1993-91109	B2	19930713		
	US 1993-163324	B2	19931206		
	US 1994-274628	A2	19940713		

OS MARPAT 128:34983
GI



I



AB Title nucleosides I (R = H, Y; R1 = benzyl, halobenzyl; R2 = H, halo, alkylamino; X1 = H, alkyl; X2 = alkylamido; X3, X4 = independently H, OH, NH2, N3, halo, Bz) were prepared as A3 adenosine receptor agonists. The present invention also provides a method of selectively activating an A3 adenosine receptor in a mammal, which method comprises acutely or chronically administering to a mammal in need of selective activation of its A3 adenosine receptor a therapeutically or prophylactically effective amount of a compound which binds with the A3 receptor so as to stimulate an A3 receptor-dependent response. Thus, N3-(3-iodobenzyl)-9-Me adenine was prepared and showed an affinity at rat brain adenosine receptors (Ki = 2.23-48.3 μM).

ST adenine prepn adenosine receptor agonist; nucleoside prepn adenosine receptor agonist

IT Nucleosides, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(adenosines; preparation of nucleosides as a adenosine receptor agonists)

IT Adenosine receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of nucleosides as a adenosine receptor agonists)

IT 162254-49-1P **163042-77-1P** 163042-82-8P 163042-85-1P
163042-86-2P 170966-19-5P 170966-21-9P 199473-28-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of nucleosides as a adenosine receptor agonists)

IT 163042-60-2P 163042-61-3P 163042-62-4P 163042-63-5P 163042-64-6P
163042-65-7P 163042-66-8P 163042-67-9P 163042-68-0P 163042-69-1P
163042-70-4P 163042-71-5P 163042-72-6P 163042-73-7P 163042-74-8P
163042-75-9P 163042-78-2P 163042-79-3P 163042-81-7P 163042-83-9P
163042-84-0P 163042-88-4P 163042-89-5P 170966-22-0P 170966-23-1P
170966-25-3P 199473-26-2P 199473-29-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nucleosides as a adenosine receptor agonists)

IT 199473-30-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of nucleosides as a adenosine receptor agonists)

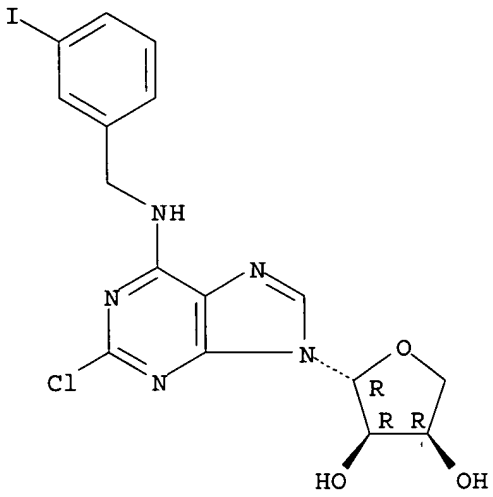
IT 9012-42-4, Adenylate cyclase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of nucleosides as a adenosine receptor agonists)

IT 87-42-3, 6-Chloropurine 538-75-0 3303-84-2 3718-88-5 5332-06-9, 4-Bromobutyronitrile 5399-87-1, 6-Chloropurine riboside 5451-40-1, 2,6-DiChloropurine 10310-21-1, 2-Amino-6-Chloropurine 23735-43-5 23788-74-1 60410-16-4 77745-22-3 152918-47-3 162254-50-4 163042-96-4 186495-36-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of nucleosides as a adenosine receptor agonists)

IT 3396-71-2P 4105-29-7P 72158-53-3P 120046-86-8P 126694-09-5P
162254-46-8P 162254-48-0P 162254-51-5P 163042-87-3P 163042-91-9P
163042-93-1P 163042-94-2P 163042-97-5P 163042-98-6P 170966-20-8P

199473-24-0P 199473-25-1P 199473-27-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nucleosides as a adenosine receptor agonists)
IT 40615-19-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of nucleosides as a adenosine receptor agonists)
IT **163042-77-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of nucleosides as a adenosine receptor agonists)
RN 163042-77-1 HCAPLUS
CN 3,4-Furandiol, 2-[2-chloro-6-[[(3-iodophenyl)methyl]amino]-9H-purin-9-yl]tetrahydro-, (2R,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:603261 HCAPLUS
DN 127:205769
ED Entered STN: 24 Sep 1997
TI 13C-1H and 13C-13C Spin-Coupling Constants in Methyl β-D-Ribofuranoside and Methyl 2-Deoxy-β-D-erythro-pentofuranoside: Correlations with Molecular Structure and Conformation
AU Church, Timothy J.; Carmichael, Ian; Serianni, Anthony S.
CS Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, 46556, USA
SO Journal of the American Chemical Society (1997), 119(38), 8946-8964
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 33-3 (Carbohydrates)
AB Me β-D-ribofuranoside (I) and Me 2-deoxy-β-D-erythro-pentofuranoside (Me 2-deoxy-β-D-ribofuranoside) (II) were synthesized with single sites of 13C-enrichment at each carbon, and a complete set of 13C-1H and 13C-13C spin-coupling consts. were obtained by 1D and 2D NMR

spectroscopy. The correlations drawn between I and II ring structure/conformation and JCH/JCC magnitude and sign in will be useful in anticipated applications of these couplings to assess furanose ring conformation/dynamics in DNA and RNA oligomers and in other biomols. containing β-D-ribo and 2-deoxy-β-D-ribo rings.

ST mol orbital conformation NMR ribofuranoside deoxyerythropentofuranoside; structure property conformation glycoside NMR

IT Conformation
(MSPR; spin coupling consts. in ribofuranoside and deoxybderythropentofuranoside and correlations with mol. structure and conformation)

IT Molecular orbital
(spin coupling consts. in ribofuranoside and deoxybderythropentofuranoside and correlations with mol. structure and conformation)

IT 97-30-3 709-50-2 13145-22-7 **17019-46-4** 29084-15-9
32445-75-3, α-D-Ribofuranose 36468-53-8, β-D-Ribofuranose
36792-88-8 53109-84-5
RL: PRP (Properties)
(spin coupling consts. in ribofuranoside and deoxybderythropentofuranoside and correlations with mol. structure and conformation)

IT 7473-45-2P 51255-18-6P 194535-64-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(spin coupling consts. in ribofuranoside and deoxybderythropentofuranoside and correlations with mol. structure and conformation)

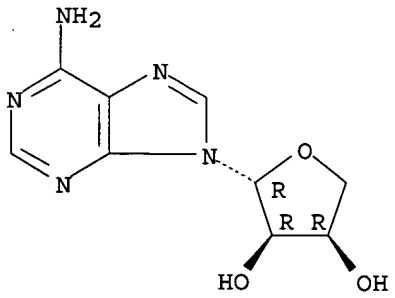
IT 194535-65-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(spin coupling consts. in ribofuranoside and deoxybderythropentofuranoside and correlations with mol. structure and conformation)

IT **17019-46-4**
RL: PRP (Properties)
(spin coupling consts. in ribofuranoside and deoxybderythropentofuranoside and correlations with mol. structure and conformation)

RN 17019-46-4 HCAPLUS

CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN

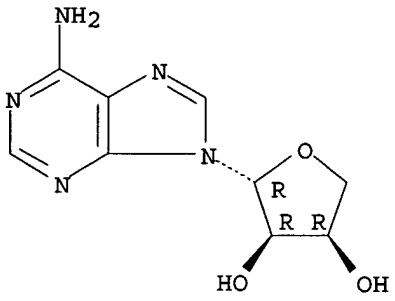
AN 1996:61304 HCAPLUS

DN 124:146708

ED Entered STN: 31 Jan 1996
TI 13C-1H Spin-Coupling Constants in the β-D-Ribofuranosyl Ring: Effect of Ring Conformation on Coupling Magnitudes
AU Podlasek, Carol A.; Stripe, Wayne A.; Carmichael, Ian; Shang, Maoyu; Basu, Bidisa; Serianni, Anthony S.
CS Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, 46556, USA
SO Journal of the American Chemical Society (1996), 118(6), 1413-25
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 33-9 (Carbohydrates)
AB Exptl. and computational methods have been used to examine the behavior of one-, two-, and three-bond 13C-1H spin-coupling consts. (1JCH, 2JCH and 3JCH, resp.) within the β-D-ribofuranosyl ring that may be potentially affected by ring conformation. Ab initio MO calcns. at the HF/6-31G* and MP2/6-31G* levels of theory were employed to assess the effect of ring conformation on mol. parameters (i.e., bond lengths, angles, and torsions) of β-D-ribofuranose (I) and Me β-D-ribofuranoside, and these data were validated through comparison to corresponding parameters obtained by X-ray crystallog. The MO-derived structural data were subsequently used to compute 1JCH, 2JCH and 3JCH values in I as a function of ring conformation. This predicted behavior was then tested exptl. through the measurement of JCH values in conformationally-rigid model compds. (aldopyranosides) containing 13C-1H coupling pathways similar to those found in specific conformers of I and was examined for consistency with previously-derived empirical rules correlating JCH with structure in carbohydrates. Available JCH data obtained on several biol.-important compds. containing β-D-ribofuranosyl rings have been interpreted in light of the new correlations with ring conformation.
ST ribofuranoside conformation structure property; ribofuranose conformation structure property; structure property conformation sugar; nucleoside ribofuranosyl ring conformation
IT Conformation and Conformers
Molecular structure-property relationship
(effect of ring conformation on 13C-1H spin-coupling magnitudes of sugars)
IT Carbohydrates and Sugars, properties
RL: PRP (Properties)
(ribofuranosyl ring; effect of ring conformation on 13C-1H spin-coupling magnitudes of sugars)
IT 58-61-7, Adenosine, properties 617-04-9, Methyl α-D-mannopyranoside 5328-63-2, Methyl β-D-arabinopyranoside 7473-45-2, Methyl β-D-ribofuranoside 18469-06-2, Methyl β-D-allopyranoside 36468-53-8, β-D-Ribofuranose 53109-84-5
RL: PRP (Properties)
(effect of ring conformation on 13C-1H spin-coupling magnitudes of sugars)
IT **17019-46-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(effect of ring conformation on 13C-1H spin-coupling magnitudes of sugars)
IT **17019-46-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(effect of ring conformation on 13C-1H spin-coupling magnitudes of sugars)

RN 17019-46-4 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:538896 HCAPLUS
DN 122:281445
ED Entered STN: 10 May 1995
TI Structure-Activity Relationships of 9-Alkyladenine and Ribose-Modified Adenosine Derivatives at Rat A3 Adenosine Receptors
AU Jacobson, Kenneth A.; Siddiqi, Suhaib M.; Olah, Mark E.; Ji, Xiao-duo; Melman, Neli; Bellamkonda, Kamala; Meshulam, Yacov; Stiles, Gary L.; Kim, Hea O.
CS Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD, 20892, USA
SO Journal of Medicinal Chemistry (1995), 38(10), 1720-35
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 1-3 (Pharmacology)
Section cross-reference(s): 33
AB 9-Alkyladenine derivs. and ribose-modified N6-benzyladenosine derivs. were synthesized in an effort to identify selective ligands for the rat A3 adenosine receptor and leads for the development of antagonists. The derivs. contained structural features previously determined to be important for A3 selectivity in adenosine derivs., such as an N6-(3-iodobenzyl) moiety, and were further substituted at the 2-position with halo, amino, or thio groups. Affinity was determined in radioligand binding assays at rat brain A3 receptors stably expressed in Chinese hamster ovary (CHO) cells, using [125I]AB-MECA (N6-(4-amino-3-iodobenzyl)adenosine-5'-(N-methyluronamide)), and at rat brain A1 and A2a receptors using [3H]-N6-PIA ((R)-N6-phenylisopropyladenosine) and [3H]CGS 21680 (2-[[[4-(2-carboxyethyl)phenyl]ethyl]amino]-5'-(N-ethylcarbamoyl)adenosine), resp. A series of N6-(3-iodobenzyl) 2-amino derivs. indicated that a small 2-alkylamino group, e.g., methylamino, was favored at A3 receptors. N6-(3-Iodobenzyl)-9-methyl-2-(methylthio)adenine was 61-fold more potent than the corresponding 2-Me ether at A3 receptors and of comparable affinity at A1 and A2a receptors, resulting in a 3-6-fold selectivity for A3 receptors. A pair of chiral N6-(3-iodobenzyl) 9-(2,3-dihydroxypropyl) derivs. showed stereoselectivity, with the R-enantiomer favored at A3 receptors by 5.7-fold. 2-Chloro-9-(β-D-erythrofuranosyl)-N6-(3-iodobenzyl)adenine had a Ki value at A3 receptors of 0.28 μM. 2-Chloro-9-[2-amino-2,3-dideoxy-β-D-5-(methylcarbamoyl)arabinofuranos

yl]-N6-(3-iodobenzyl)adenine was moderately selective for A1 and A3 vs A2a receptors. A 3'-deoxy analog of a highly A3-selective adenosine derivative retained selectivity in binding and was a full agonist in the inhibition of adenylyl cyclase mediated via cloned rat A3 receptors expressed in CHO cells. The 3'-OH and 4'-CH_2OH groups of adenosine are not required for activation at A3 receptors. A number of 2',3'-dideoxyadenosines and 9-acyclic-substituted adenines inhibited adenylyl cyclase at the allosteric "P" site.

ST adenine ribose deriv MSBAR adenosine receptor

IT Molecular structure-biological activity relationship
(adenosine A3-agonist; structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

IT Receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(purinergic A3, structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

IT 10147-12-3 79813-69-7 109292-91-3 135394-08-0 152918-18-8 163181-33-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

IT 163042-96-4
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

IT 163042-66-8P **163042-77-1P** 163042-82-8P 163042-83-9P 163042-85-1P 163042-86-2P 163042-87-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

IT 58-61-7DP, Adenosine, ribose-modified derivs. 73-24-5DP, Adenine, alkyl derivs. 163042-60-2P 163042-61-3P 163042-62-4P 163042-63-5P 163042-64-6P 163042-65-7P 163042-67-9P 163042-68-0P 163042-69-1P 163042-70-4P 163042-71-5P 163042-72-6P 163042-73-7P 163042-74-8P 163042-75-9P 163042-76-0P 163042-78-2P 163042-79-3P 163042-80-6P 163042-81-7P 163042-84-0P 163042-88-4P 163042-89-5P 163042-90-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

IT 58-61-7, Adenosine, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

IT 64-69-7, Iodoacetic acid 87-42-3 107-10-8, n-Propylamine, reactions 111-26-2, n-Hexylamine 583-50-6, D-Erythrose 624-76-0, 2-Iodoethanol 1005-56-7, Phenoxythiocarbonyl chloride 1191-99-7, 2,3-Dihydrofuran 3718-88-5, 3-Iodobenzylamine hydrochloride 5332-06-9, 4-Bromobutyronitrile 5451-40-1, 2,6-Dichloropurine 5680-79-5, Glycine methyl ester hydrochloride 6022-96-4 10310-21-1, 6-Chloroguanine 69304-37-6, 1,3-Dichloro-1,1,3,3-tetraisopropyldisiloxane
RL: RCT (Reactant); RACT (Reactant or reagent)

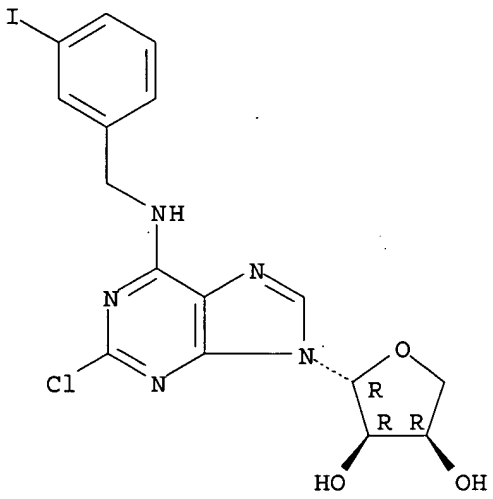
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

IT 3396-71-2P 4105-29-7P 72158-53-3P 112288-77-4P 120046-86-8P 126694-09-5P 163042-91-9P 163042-92-0P 163042-93-1P 163042-94-2P 163042-95-3P 163042-97-5P 163042-98-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

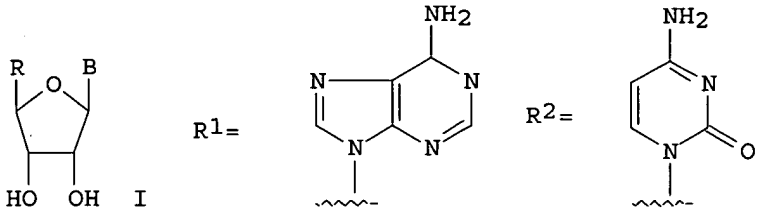
IT **163042-77-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

RN 163042-77-1 HCAPLUS
CN 3,4-Furandiol, 2-[2-chloro-6-[[(3-iodophenyl)methyl]amino]-9H-purin-9-yl]tetrahydro-, (2R,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:152266 HCAPLUS
DN 116:152266
ED Entered STN: 17 Apr 1992
TI (13C)-Substituted erythronucleosides: synthesis and conformational analysis by proton and carbon-13 NMR spectroscopy
AU Kline, Paul C.; Serianni, Anthony S.
CS Dep. Chem. Biochem., Univ. Notre Dame, Notre Dame, IN, 46556, USA
SO Journal of Organic Chemistry (1992), 57(6), 1772-7
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 33-9 (Carbohydrates)
Section cross-reference(s): 22
GI



AB The erythrofuranosyl nucleosides, e.g. I (R = H, CH2OH, B = R1,R2), were synthesized with and without 13C-substitution at C1' of the furanose ring. 13C 1H NMR spectra of I were interpreted, in the latter case with the assistance of spectral simulation, and 1H-1H, 13C-1H, and 13C-13C spin couplings were used to assess furanose conformation. 3JHH Data in 2H2O were treated by computer to determine the preferred conformers, their puckering amplitudes, and their mole fractions in soluble, and JCH data were used to complement this anal.

ST erythrofuranosyl nucleoside prepn conformation NMR

IT Conformation and Conformers
(of erythrofuranosyl nucleosides, NMR in relation to)

IT Nucleosides, properties
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(erythrofuranosyl, preparation and conformation of, NMR in relation to)

IT 583-50-6, D-Erythrose
RL: RCT (Reactant); RACT (Reactant or reagent)
(acetylation of)

IT 70849-19-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with adenine)

IT 66-22-8, Uracil, reactions 4005-49-6, N6-Benzoyladenine 14631-20-0, N4-Acetylcytosine 21967-06-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling of, with erythrofuranose derivs.)

IT 58-61-7P, Adenosine, preparation 65-46-3P, Cytidine 118-00-3P, Guanosine, preparation **17019-46-4P** 40653-40-5P 63713-91-7P 138874-51-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation of, NMR in relation to)

IT 66757-61-7P 66757-62-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and coupling of, with nucleoside basis)

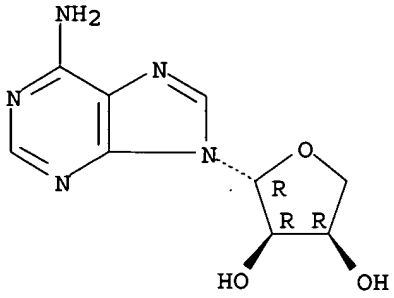
IT **138722-89-1P** 138722-90-4P 138722-91-5P 138722-92-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **17019-46-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and conformation of, NMR in relation to)

RN 17019-46-4 HCAPLUS

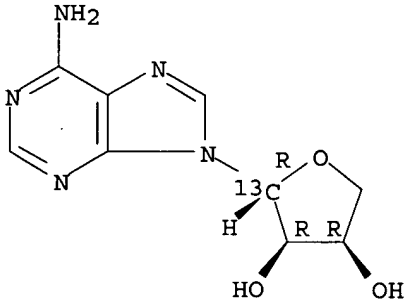
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

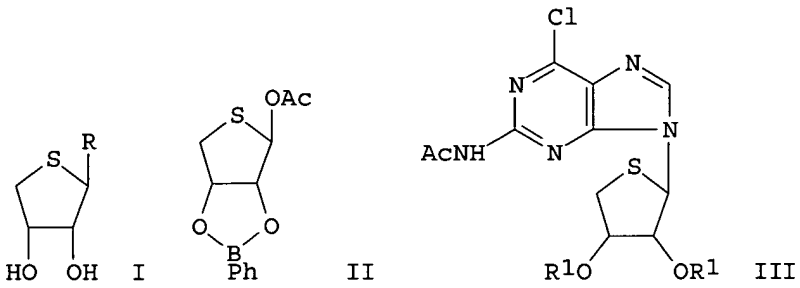


IT **138722-89-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 138722-89-1 HCAPLUS
CN 3,4-Furandiol-2-13C, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:22947 HCAPLUS
DN 100:22947
ED Entered STN: 12 May 1984
TI Thio sugars - Part 9. Antiviral nucleosides from 4-thio-DL-erythrofuranose and purines and other fused pyrimidines
AU McCormick, Joan E.; McElhinney, R. S.
CS Lab. Med. Res. Counc., Trinity Coll., Dublin, Ire.
SO Proceedings of the Royal Irish Academy, Section B: Biological, Geological and Chemical Science (1983), 83 B(1-16), 125-38
CODEN: PRIBAN; ISSN: 0035-8983
DT Journal
LA English
CC 33-9 (Carbohydrates)
GI



AB Nucleosides I [R = substituted purin-9-yl, 2-(o-propoxyphenyl)-8-azahypoxanthin-9-yl, (un)substituted 2,4-dioxo-1,2,3,4-tetrahydroquinazolin-1(or 3)-yl] and 2',3'-seco-analogs of some of them were prepared Thus, 2-acetamido-6-chloropurine was glycosylated with II (by fusion in the presence of p-MeC6H4SO3H) to give 45% nucleoside III (R12 = PhB), which was deboronated to give 90% III (R1 = H). Application of various exptl. conditions for purine glycosylation with 4-thioerythrofuranose derivs. was also studied.

ST nucleoside thioerythrofuranose purine pyrimidine; quinazoline thioerythrofuranose nucleoside; glycosylation purine thioerythrofuranose; azahypoxanthine nucleoside thioerythrofuranose

IT Glycosidation
(of purines with thioerythrofuranose derivs.)

IT Nucleosides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from thioerthrofuranose and purines and other fusion pyrimidines)

IT 88145-77-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzoylation of)

IT 78755-94-9
RL: PROC (Process)
(conversion of, to fluoromethylenedione)

IT 88198-62-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(deboronation of)

IT 62729-48-0 66944-17-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(glycosylation by, of purine derivative)

IT 88145-81-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)

IT 66929-18-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)

IT 88145-78-2P 88145-84-0P 88145-87-3P 88145-88-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deboronation of)

IT 88145-80-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

IT 1640-60-4P 16353-27-8P 88145-86-2P 88145-89-5P 88145-90-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and thioerythrofuranosylation of)

IT **88145-69-1P** 88145-70-4P 88145-72-6P 88145-73-7P
88145-74-8P 88145-75-9P 88145-76-0P 88145-79-3P
88145-82-8P 88145-83-9P 88145-85-1P 88145-91-9P 88145-92-0P
88145-93-1P 88145-94-2P 88145-95-3P 88145-96-4P 88145-97-5P
88145-98-6P 88145-99-7P 88146-00-3P 88146-01-4P 88146-02-5P
88146-03-6P 88146-04-7P 88146-05-8P 88146-06-9P 88146-07-0P
88146-08-1P 88146-09-2P 88146-10-5P 88146-11-6P 88146-12-7P
88156-47-2P 88156-48-3P 88156-49-4P 88198-63-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 74-93-1, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (thioerythrofuranosyl)purine derivative)

IT 77594-20-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chloropurine)

IT 75-04-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thioerythrofuranosyl purine derivative)

IT 87-42-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with triacetoxythiapantane)

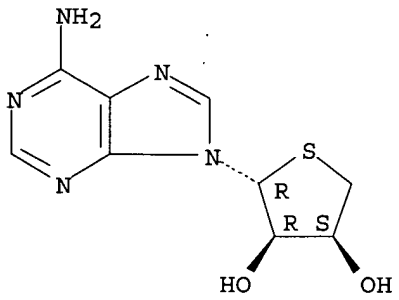
IT 68-94-0 4005-49-6 7602-01-9 37762-06-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(thioerythrofuranosylation of)

IT 683-67-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(trimethylsilylation of, in synthesis of (thioerythrofuranosyl)propylamine)

IT **88145-69-1P 88145-74-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

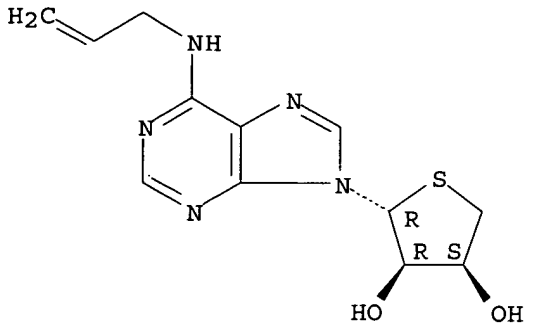
RN 88145-69-1 HCAPLUS
CN 3,4-Thiophenediol, 2-(6-amino-9H-purin-9-yl)tetrahydro-,
(2α,3β,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

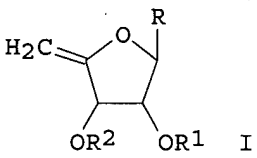


RN 88145-74-8 HCAPLUS
CN 3,4-Thiophenediol, tetrahydro-2-[6-(2-propenylamino)-9H-purin-9-yl]-,
(2α,3β,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L19 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:454117 HCAPLUS
DN 99:54117
ED Entered STN: 12 May 1984
TI Synthesis, structure, and reactivity of selenoxides derived from ribose and adenosine: new method for access to C(4')-C(5') unsaturated ribofuranosides
AU Boullais, C.; Zylber, N.; Zylber, J.; Guilhem, J.; Gaudemer, A.
CS Groupe Rech., CNRS, Thiais, 94320, Fr.
SO Tetrahedron (1983), 39(5), 759-65
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA French
CC 33-9 (Carbohydrates)
GI

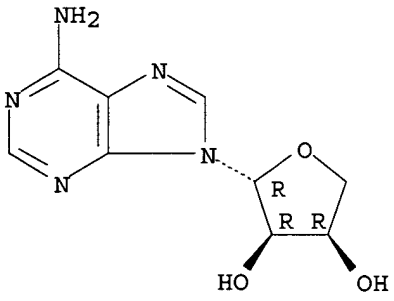


I

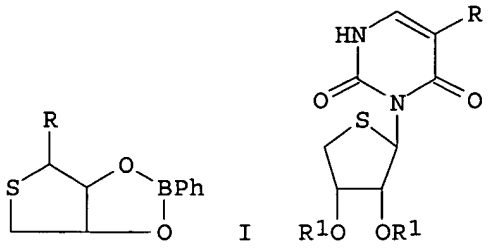
AB A new method for the introduction of an exocyclic double bond at C(4)-C(5) of ribose or adenosine to give I (R = OMe, adenyl; R1 = R2 = H; R1R2 = CMe2) uses the easy conversion of selenoxides to the corresponding alkenes by thermal elimination. Ribose, adenosine and their 2,3'-O-isopropylidene derivs. have been converted to their 5-phenylselenides and adenosine also to its o-nitrophenylselenide which were oxidized to the selenoxides. Thermal eliminations of the selenoxides were carried out at 60-80°, the rates depending on the solvent, the substituents at C(1) and C(3) and the configuration at the Se chiral center.
ST erythropentenofuranoside; erythropentenofuranosyladenine; adenine erythropentenofuranosyl; deoxyphenylselenoxyribofuranose prepn elimination
IT 69938-31-4P 69938-32-5P 86520-92-5P 86520-93-6P 86539-95-9P 86549-39-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and elimination of phenylselenyl group from)
IT 86520-89-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and of)

IT 86520-87-8P 86520-88-9P 86520-91-4P 86520-94-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
IT **17019-46-4P** 53109-84-5P 79849-80-2P 79849-81-3P
86520-90-3P 86560-90-9P 86560-91-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 51694-22-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with adenosine)
IT 892-48-8 4137-56-8 24514-56-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with di-Ph diselenide)
IT 58-61-7, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitrophenylselenocyanate)
IT **17019-46-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 17019-46-4 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L19 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:597852 HCAPLUS
DN 89:197852
ED Entered STN: 12 May 1984
TI Thio sugars. Part 3. 4-Thiotetrofuranose nucleosides
AU McCormick, Joan E.; McElhinney, R. Stanley
CS Lab. MRC Ireland, Trinity Coll., Dublin, Ire.
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1978), (5), 500-5
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
CC 33-7 (Carbohydrates)
Section cross-reference(s): 28, 29
GI



AB Boronates I (R = 6-chloro-, 2,6-dichloropurin-9-yl, theophyllin-7-yl) and II (R = H, Me, F, Br, iodo, R12 = BPh) were prepared (31-65%) by condensation of acetate I (R = OAc) with appropriate purines in the presence of 4-MeC6H4SO3H (MeNO2, 100°, 10 min- 1 h), and with uracils [bis(Me3Si) derivs.] in the presence of SnCl4 (CH2Cl2, room temperature)
resp. Deboronation of II (R, R1 as before) with HO(CH2)3OH gave 58-70% of corresponding nucleosides II (R1 = OH).

ST acetylthiofuranose phenylboronate condensation purine; uracylthiofuranose boronate deboronation; nucleoside thiotetrafuranose

IT Condensation reaction
(of acetylthiofuranose phenylboronate with dichloropurine, theophylline, and uracil derivs.)

IT Elimination reaction
(deboronation, of thiofuranosylpurine and -uracil phenylboronates)

IT Nucleosides, preparation
(thiofuranose, preparation of, by condensation of acetylthiofuranose phenylboronate with dichloropurine, theophylline, and uracil derivs.)

IT 104-15-4, uses and miscellaneous 645-15-8
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for condensation of acetylthiofuranose phenylboronate with dichloropurine)

IT 58-55-9, reactions 3442-82-8 3444-09-5 5451-40-1 58138-78-6 66818-26-6 68116-15-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with acetylthiofuranose phenylboronate)

IT 68128-78-9 68128-79-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with dichloropurine and theophylline)

IT 54-85-3 6610-29-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with oxidation products of purinylthiofuranose derivs.)

IT 102-09-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization by, of thiofuranosylpurine and -uracil derivative)

IT 68116-19-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)

IT 68116-14-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)

IT **68116-24-5P** 68128-81-4P 68128-87-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, anhydro(thiofuranosyl)uracil by)

IT 68116-11-0P 68116-12-1P 68116-13-2P 68116-17-6P 68116-27-8P
68116-28-9P 68116-29-0P 68116-30-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deboronation of)

IT 68128-80-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dechlorination of, by benzylamine and alcs.)

IT 68116-21-2P 68116-22-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and periodate oxidation of)

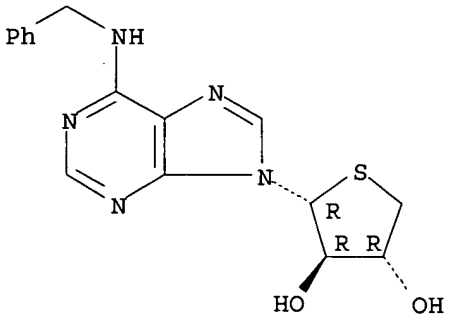
IT 66929-21-3P 66929-22-4P 68116-16-5P **68116-18-7P**
68116-20-1P 68116-23-4P 68116-25-6P 68116-26-7P 68128-82-5P
68128-83-6P 68128-84-7P 68128-85-8P 68128-86-9P 68136-80-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 67-56-1, reactions 100-46-9, reactions 100-51-6, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with chloropurinylthiofuranose)

IT **68116-24-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, anhydro(thiofuranosyl)uracil by)

RN 68116-24-5 HCAPLUS
CN 3,4-Thiophenediol, tetrahydro-2-[6-[(phenylmethyl)amino]-9H-purin-9-yl]-, [2R-(2α,3β,4α)]- (9CI) (CA INDEX NAME)

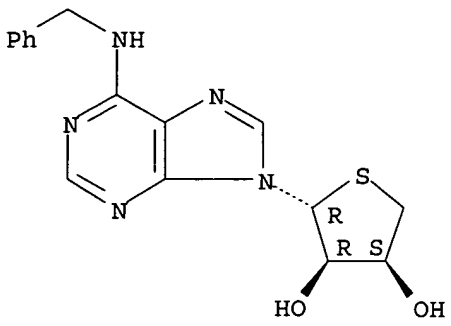
Absolute stereochemistry.



IT **68116-18-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

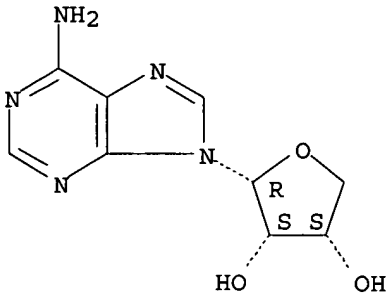
RN 68116-18-7 HCAPLUS
CN 3,4-Thiophenediol, tetrahydro-2-[6-[(phenylmethyl)amino]-9H-purin-9-yl]-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



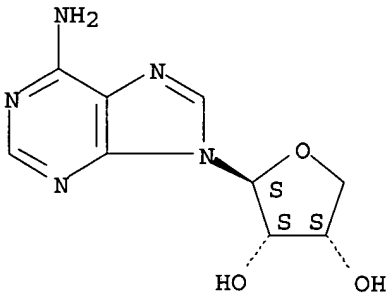
L19 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:58203 HCAPLUS
DN 70:58203
ED Entered STN: 12 May 1984
TI Preparation of nucleosides via isopropylidene sugar derivatives. IV. Synthesis of 9-[α(and β)-L-erythro furanosyl]adenine
AU Lerner, Leon M.
CS Downstate Med. Center, State Univ. of New York, Brooklyn, NY, USA
SO Journal of Organic Chemistry (1969), 34(1), 101-3
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
CC 33 (Carbohydrates)
AB 2,3-O-Isopropylidene-β-L-erythrofuranosyl chloride was condensed with 6-benzamidochloromercuripurine and the blocking groups were removed to yield the anomers of 9-L-erythrofuranosyladenine which were separated by column chromatography. In all expts. the β anomer was the main product, leading to the conclusion that this condensation proceeded by an SN1 mechanism.
ST erythrofuranosyladenosine; furanosyladenosines erythro; adenosines erythrofuranosyl
IT Nucleosides
RL: SPN (Synthetic preparation); PREP (Preparation)
(erythrofuranosyl, preparation of)
IT **14266-04-7P 17019-48-6P** 18031-21-5P
18031-22-6P 18031-25-9P 18031-26-0P **18031-27-1P**
18031-43-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **14266-04-7P 17019-48-6P 18031-22-6P**
18031-27-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14266-04-7 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3α,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 17019-48-6 HCAPLUS
CN Adenine, 9-β-L-erythrofuranosyl- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

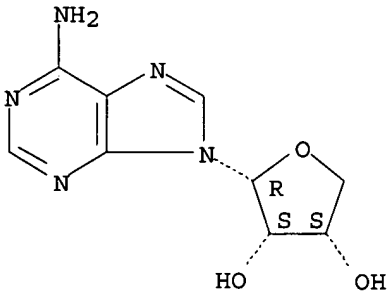


RN 18031-22-6 HCAPLUS
CN Adenine, 9-α-L-erythrofuranosyl-, monopicrate (8CI) (CA INDEX NAME)

CM 1

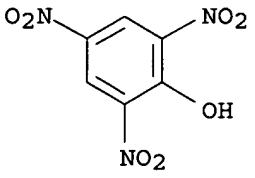
CRN 14266-04-7
CMF C9 H11 N5 O3

Absolute stereochemistry.



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7

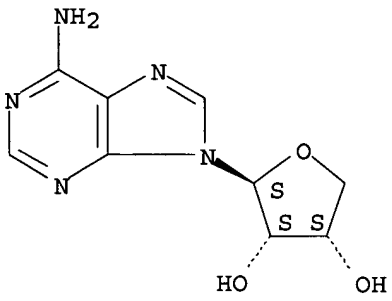


RN 18031-27-1 HCAPLUS
CN Adenine, 9-β-L-erythrofuranosyl-, monopicrate (8CI) (CA INDEX NAME)

CM 1

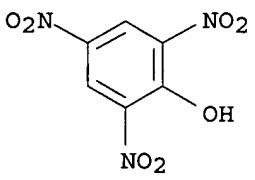
CRN 17019-48-6
CMF C9 H11 N5 O3

Absolute stereochemistry.



CM 2

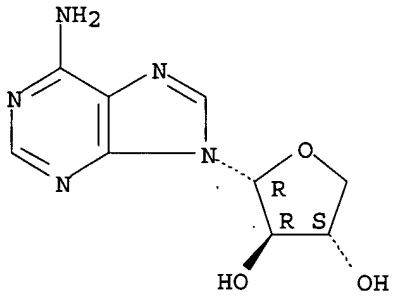
CRN 88-89-1
CMF C6 H3 N3 O7



L19 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:482354 HCAPLUS
DN 67:82354
ED Entered STN: 12 May 1984
TI Synthesis of tetrose nucleosides. I. Adenine nucleosides of erythrose and threose
AU Murray, Daniel Harry; Prokop, John
CS Univ. of New York, Buffalo, NY, USA
SO Journal of Pharmaceutical Sciences (1967), 56(7), 865-70
CODEN: JPMSAE; ISSN: 0022-3549
DT Journal

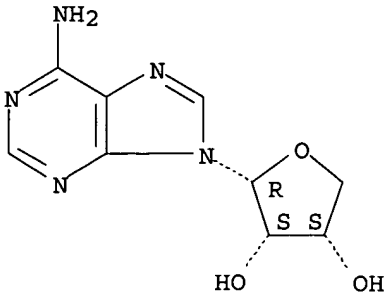
LA English
CC 33 (Carbohydrates)
AB D- and L-Erythrose and D- and L-threose were individually converted to their triacetates which were condensed with chloromercuri-6-benzamidopurine in the presence of TiCl4. After deacylation, the four crude mixts. of anomeric nucleosides were each resolved on a strong anion-exchange resin, leading to the isolation of all eight possible 9-tetrafuranosyladenines. The anomeric configurational assignments were made by consideration of the mechanism of nucleoside condensation and by Hudson's rules (H. and Jackson, CA 31: 53291) of isorotation. Preliminary results of tests for biol. activity with Streptococcus faecalis and with adenosine deaminase are reported. 18 references.
ST PROKOP J; MURRAY D H; TETROSE NUCLEOSIDES; ADENINE NUCLEOSIDES; NUCLEOSIDES TETROSE
IT **14266-03-6P 14266-04-7P 14434-23-2P**
17019-45-3P 17019-46-4P 17019-48-6P
17019-50-0P 17019-54-4P 17117-99-6P 17117-99-6P
17117-99-6P 17117-99-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **14266-03-6P 14266-04-7P 14434-23-2P**
17019-45-3P 17019-46-4P 17019-48-6P
17019-50-0P 17019-54-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14266-03-6 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, (2R,3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



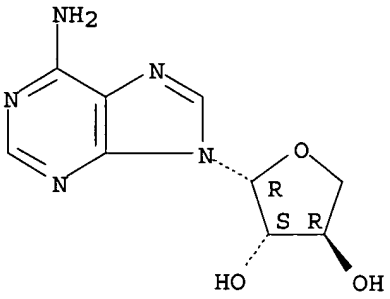
RN 14266-04-7 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3α,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



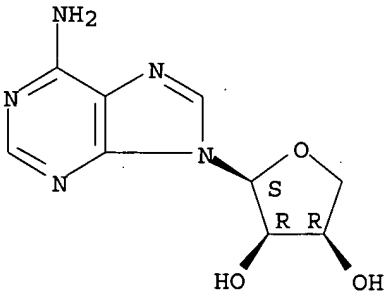
RN 14434-23-2 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3α,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



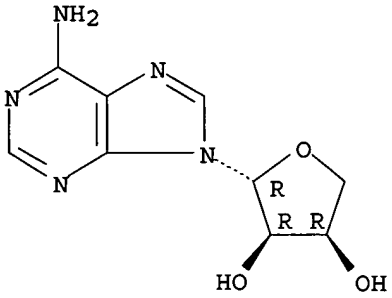
RN 17019-45-3 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, (2S,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



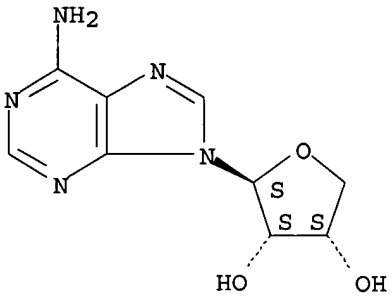
RN 17019-46-4 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



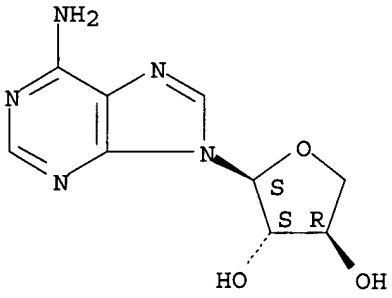
RN 17019-48-6 HCAPLUS
CN Adenine, 9-β-L-erythrofuranosyl- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



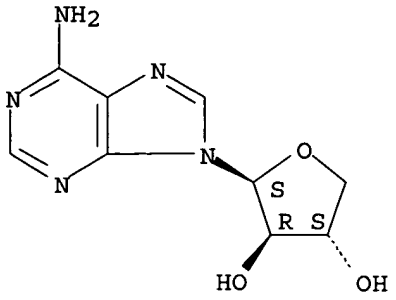
RN 17019-50-0 HCAPLUS
CN Adenine, 9-α-D-threofuranosyl- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 17019-54-4 HCAPLUS
CN Adenine, 9-β-L-threofuranosyl- (8CI) (CA INDEX NAME)

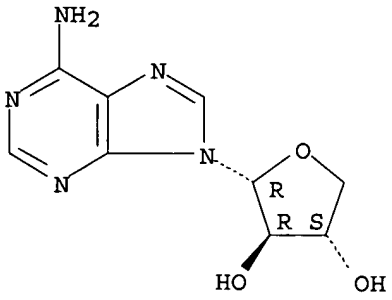
Absolute stereochemistry.



L19 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:470707 HCAPLUS
DN 67:70707
ED Entered STN: 12 May 1984
TI Role of the 5'-hydroxyl group of adenosine in determining substrate specificity for adenosine deaminase
AU Bloch, Alexander; Robins, Morris J.; McCarthy, James R., Jr.
CS Roswell Park Mem. Inst., Buffalo, NY, USA
SO Journal of Medicinal Chemistry (1967), 10(5), 908-12
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 3 (Enzymes)
AB The relation between structural alterations in the carbohydrate moiety of adenosine and the resulting changes in substrate activity was examined with adenosine deaminase. Of the 43 analogs studied, 16 were deaminated, all of them at slower rates than the natural substrate. With the exception of adenosine 2'- or 3'-monophosphate, modifications at the 2' or 3' positions, including the simultaneous removal of the 2'-and 3'-hydroxyl groups or changes in their steric configuration, did not abolish substrate activity. Replacement of the bridge O with S allowed deamination, but modifications at the 1' position prevented it. Replacement or substitution of the 5'-hydroxyl group with a variety of other groups, or removal of the 4'-hydroxymethyl group, invariably led to loss of substrate activity. Very low activity was retained when an amino group replaced the 5'-hydroxyl group, or when, in the absence of the 5'-hydroxyl, an hydroxyl group was present at carbon 3' in configuration cis to the base moiety. These data show that the 2'- or 3'-hydroxyl groups of adenosine are not required for substrate activity, but that the 5'-hydroxyl group is essential for binding to the enzyme unless its function can be assumed to a very limited extent by an amino or possibly other hydrogen-bonding groups, or by an hydroxyl group at the 3' position cis to the base. The implication of these observations for the design of adenosine analogs of interest in chemotherapy is discussed.
ST SUBSTRATE SPECIFICITY DEAMINASE; DEAMINASE ADENOSINE HYDROXYLS; ADENOSINE DEAMINASE HYDROXYLS; HYDROXYLS ADENOSINE DEAMINASE
IT Molecular structure-biological activity relationships
(adenosine deaminase substrate, adenosine 5'-hydroxyl group in)
IT Adenine, 9-β-D-fructofuranosyl-
Adenosine, 5'-deoxy-5'-(methylthio)-
RL: BIOL (Biological study)
(as adenosine deaminase substrate)
IT 3,6-Dioxabicyclo[3.1.0]hexane, sugar derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

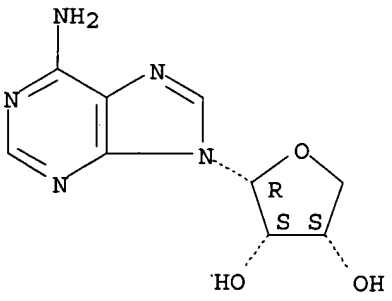
IT 58-61-7, biological studies
RL: BIOL (Biological study)
(5'-hydroxyl group of, as adenosine deaminase substrate requirement)
IT 61-19-8, biological studies 72-90-2 73-03-0 84-21-9 130-49-4
362-75-4 958-09-8 1874-54-0 2140-25-2 2140-79-6 2500-80-3
2504-55-4 4005-33-8 4097-22-7 4152-65-2 4152-76-5 4754-39-6
5536-17-4 6612-70-0 6612-73-3 6698-26-6 6746-31-2 7057-48-9
7697-49-6 **14266-03-6 14266-04-7** 14365-44-7
14365-45-8 14426-54-1 **14434-23-2** 14585-60-5
17019-46-4 17318-24-0 17434-44-5 17434-50-3 17434-51-4
17434-52-5 17434-53-6 17434-54-7 17863-53-5 18031-28-2
RL: BIOL (Biological study)
(as adenosine deaminase substrate)
IT 9026-93-1, Deaminases, adenosine
(substrate specificity of, adenosine 5'-hydroxyl group in)
IT **14266-03-6 14266-04-7 14434-23-2**
17019-46-4
RL: BIOL (Biological study)
(as adenosine deaminase substrate)
RN 14266-03-6 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, (2R,3R,4S)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



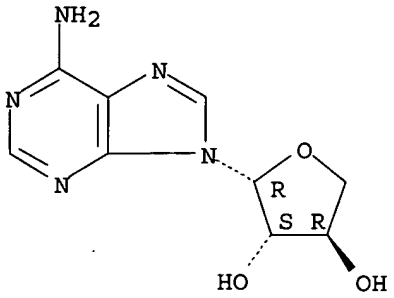
RN 14266-04-7 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-
(2α,3α,4α)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



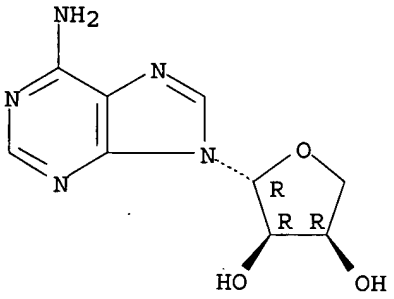
RN 14434-23-2 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-
(2α,3α,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 17019-46-4 HCAPLUS
CN 3,4-Furandiol, 2-(6-amino-9H-purin-9-yl)tetrahydro-, [2R-(2α,3β,4β)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> b uspatall
FILE 'USPATFULL' ENTERED AT 16:29:01 ON 25 MAR 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 16:29:01 ON 25 MAR 2004
CA INDEXING COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

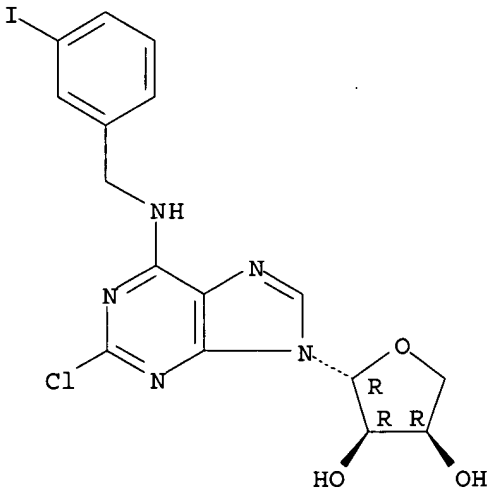
=> d bib abs hitstr tot l20

L20 ANSWER 1 OF 1 USPATFULL on STN
AN 97:107061 USPATFULL
TI A.sub.3 adenosine receptor agonists
IN Jacobson, Kenneth A., Silver Spring, MD, United States
Jeong, Heaok Kim, Rockville, MD, United States
Siddiqi, Suhaib M., Gaithersburg, MD, United States
Johnson, Carl R., Detroit, MI, United States
Secrist, III, John A., Birmingham, AL, United States
Tiwari, Kamal N., Birmingham, AL, United States
PA The United States of America as represented by the Department of Health and Human Services, Washington, DC, United States (U.S. government)
PI US 5688774 19971118
AI US 1995-396111 19950228 (8)
RLI Continuation-in-part of Ser. No. US 1994-274628, filed on 13 Jul 1994

which is a continuation-in-part of Ser. No. US 1993-163324, filed on 6 Dec 1993, now abandoned which is a continuation-in-part of Ser. No. US 1993-91109, filed on 13 Jul 1993, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Kunz, Gary L.
LREP Leydig, Voit & Mayer, Ltd.
CLMN Number of Claims: 16
ECL Exemplary Claim: 1
DRWN 13 Drawing Figure(s); 13 Drawing Page(s)
LN.CNT 2283
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention provides A.sub.3 selective agonists, particularly, adenine compounds having selected substituents at the 2, 6, and 9 positions, and related substituted compounds, particularly those containing substituents on the benzyl and/or uronamide groups, as well as pharmaceutical compositions containing such compounds. The present invention also provides a method of selectively activating an A.sub.3 adenosine receptor in a mammal, which method comprises acutely or chronically administering to a mammal in need of selective activation of its A.sub.3 adenosine receptor a therapeutically or prophylactically effective amount of a compound which binds with the A.sub.3 receptor so as to stimulate an A.sub.3 receptor-dependent response.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **163042-77-1P**
(preparation of nucleosides as a adenosine receptor agonists)
RN 163042-77-1 USPATFULL
CN 3,4-Furandiol, 2-[2-chloro-6-[[(3-iodophenyl)methyl]amino]-9H-purin-9-yl]tetrahydro-, (2R,3R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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